Chapter 2: Crystal symmetry

Crystal symmetry: crystals possess symmetry when perform any of symmetry operation and repetition of crystal face could occur.

Symmetry operation

1. Translation
2. Rotation
3. Reflection
4. Combination of translation and rotation
5. Combination of translation and reflection

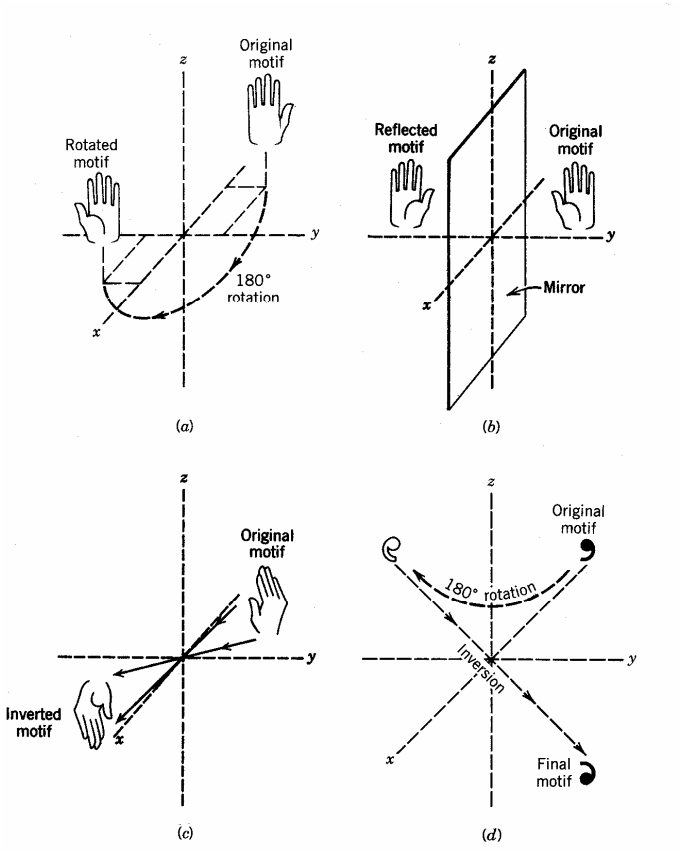
Symmetry elements

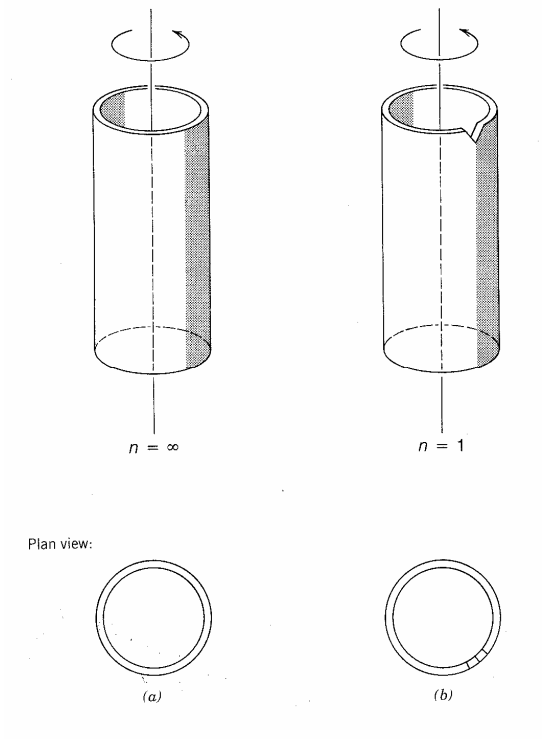
1. **A rotation axis**: An imaginary line through a crystal, which the crystal may be rotated and repeat itself in appearance (1), 2, 3, 4, or 6 times during the complete rotation (360°).

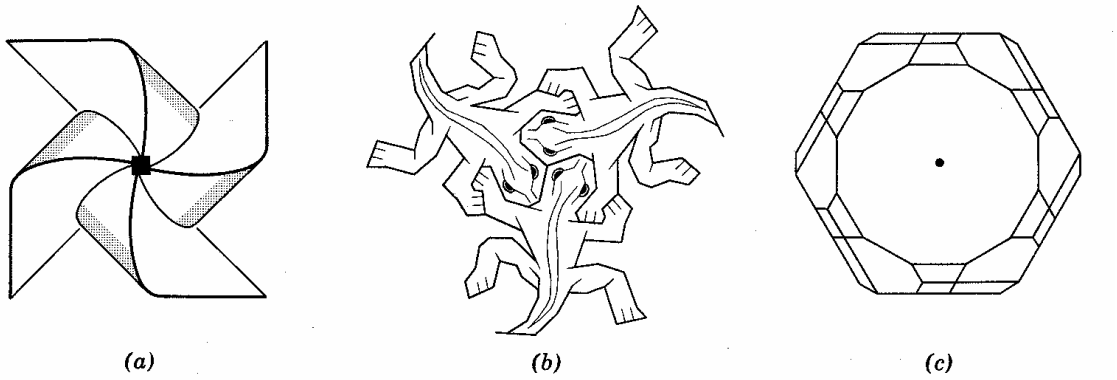
2. **A mirror plane**: An imaginary plane that divides a crystal into halves, each of which, in a perfectly developed crystal, is a mirror image to the other.

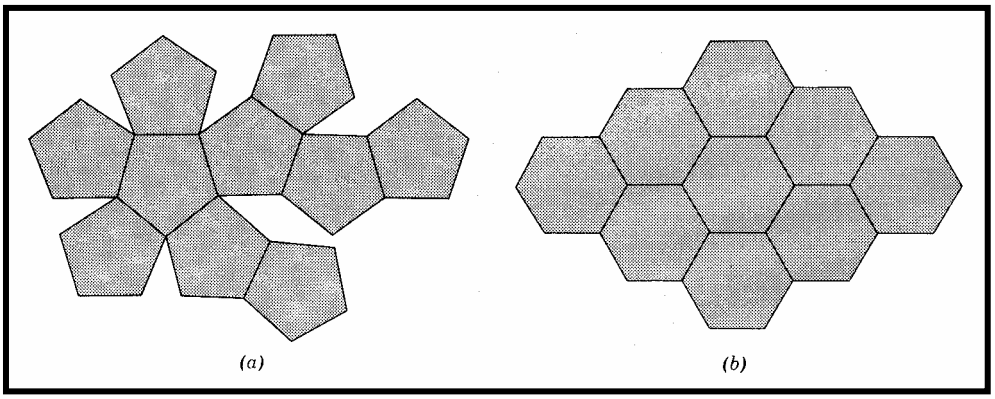
3. **A centre of symmetry**: A symmetry element that present in a crystal if an imaginary line can be passed from any point on its surface through its centre and a similar point is found on the line at an equal distance beyond the centre.

4. **A rotoinversion axis**: An imaginary line that relates to rotation about an axis with inversion









5-fold symmetry leads to gaps in the pattern

Honey comb pattern with 6-fold axes $\perp$ to the page

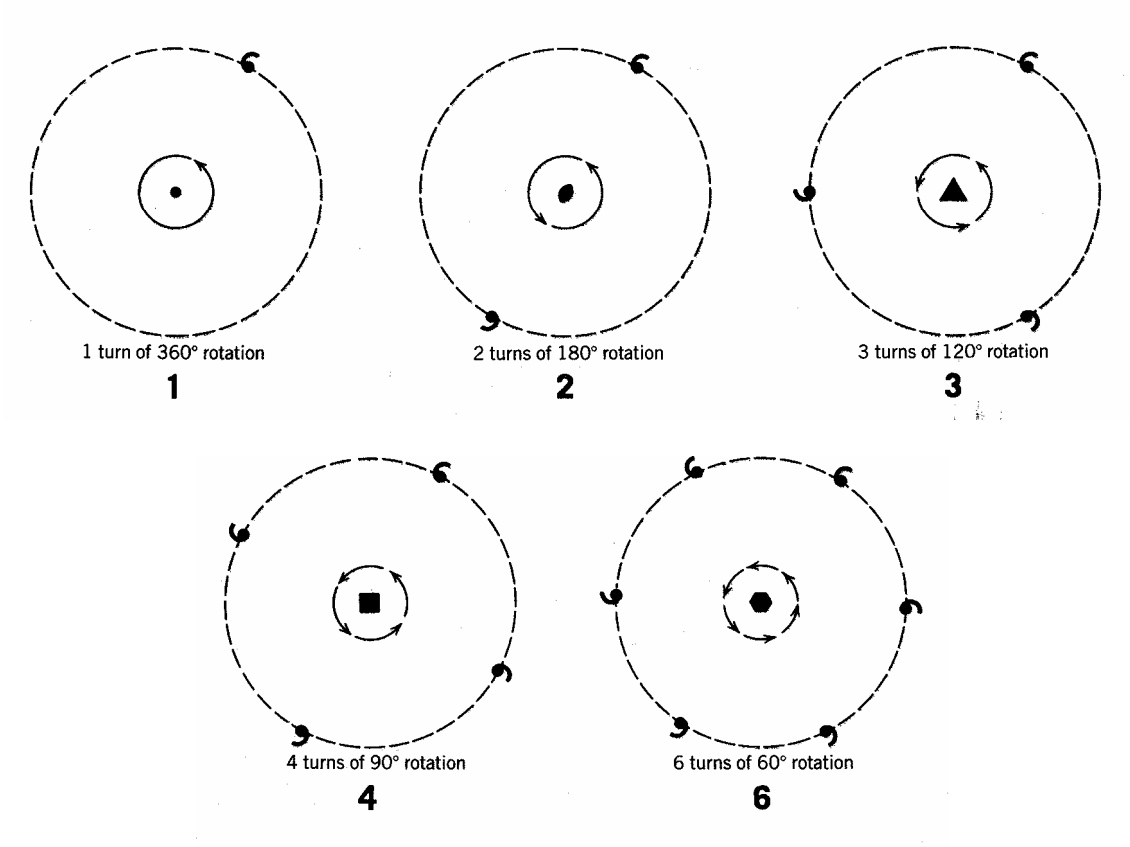
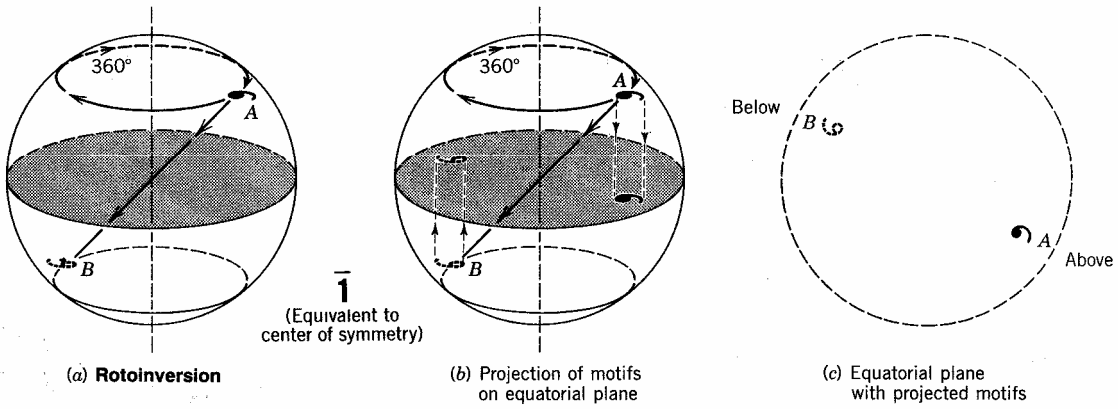


FIG. 2.11. *(a)* Illustration of an operation of rotoinversion, consisting of 360° rotation and subsequent inversion through the center of the globe. *(b)* Projection of the two motif units (*A* and *B*) from the outer skin of the globe onto the equatorial plane. *(c)* Location of the projected motifs on the equatorial plane (see also Fig. 2.12).



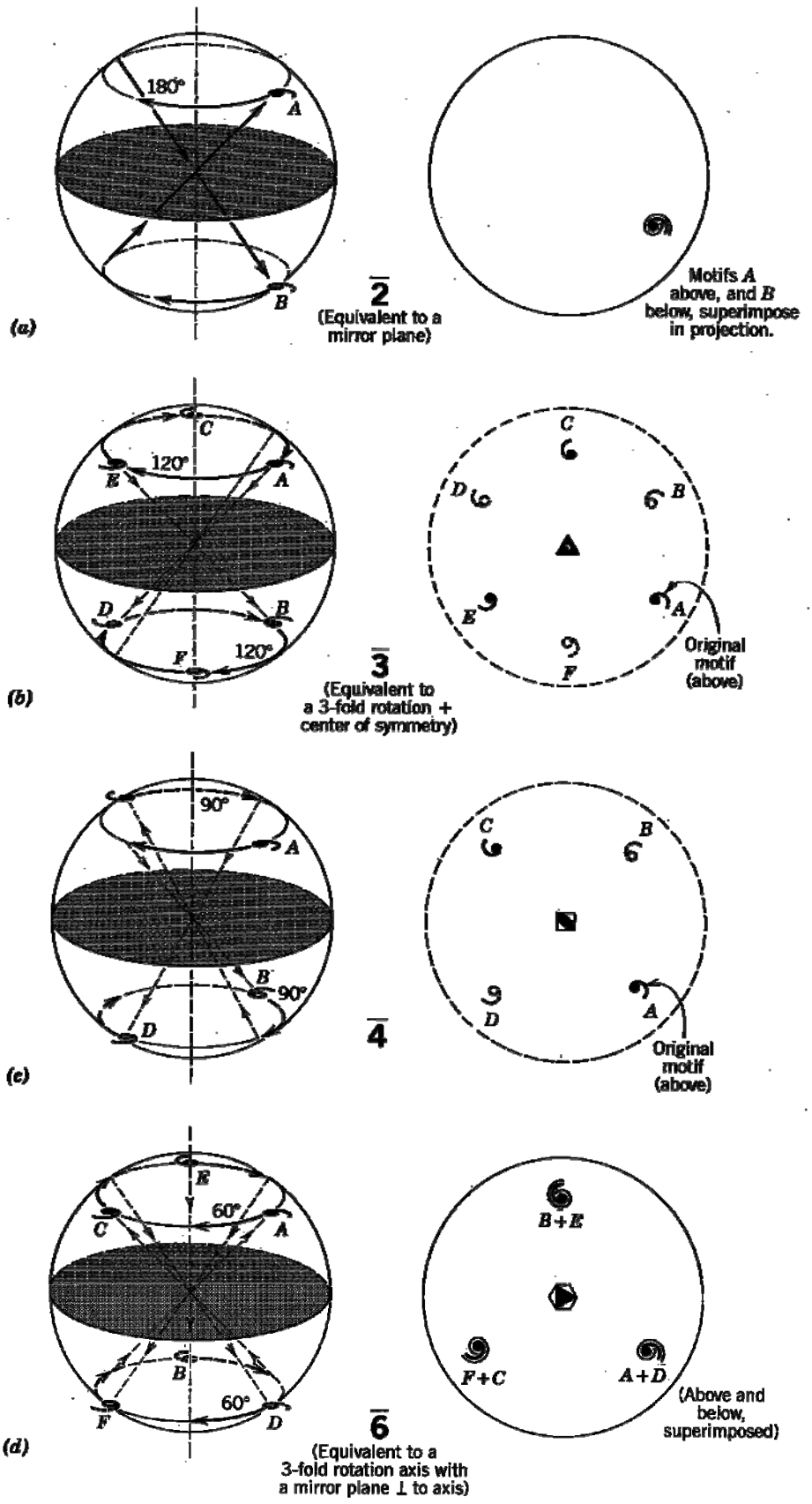
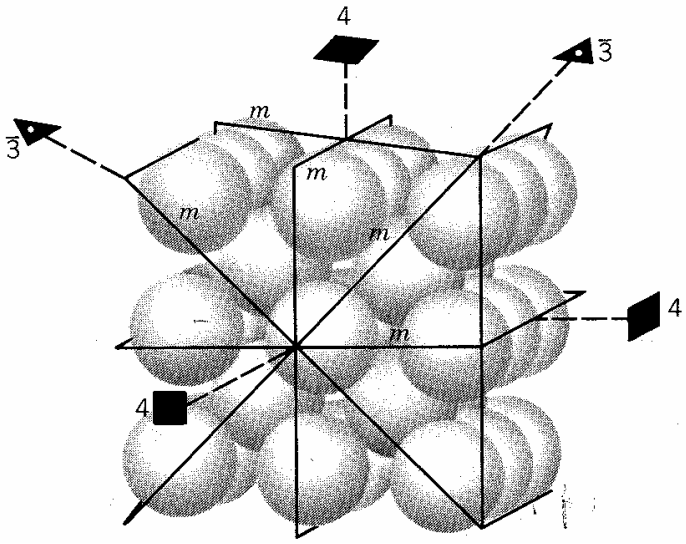
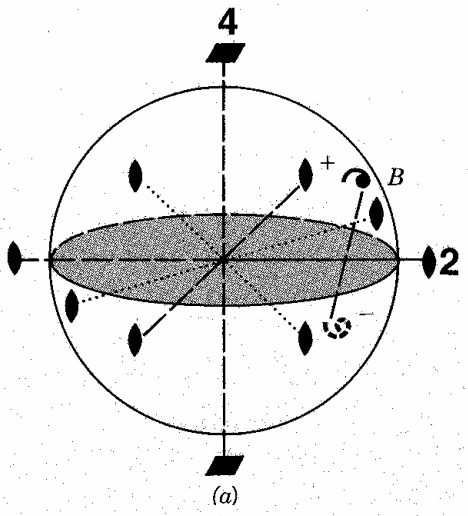
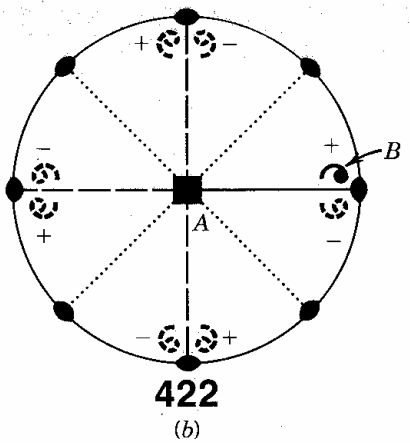


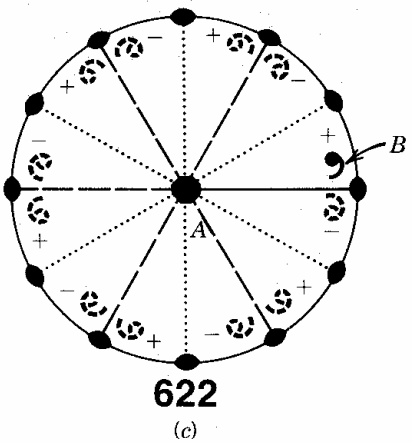
FIG. 2.12. Illustration of operations of rotoinversion on motif units. To go from unit *A* to *B* (to *C*, etc.) involves rotation through an angle α (360°, 180°, 120°, 90°, or 60°) as well as inversion through the center (see Fig. 2.11 for illustration of projection scheme).

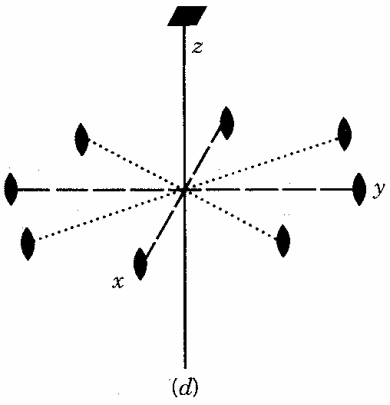
Combinations of rotations

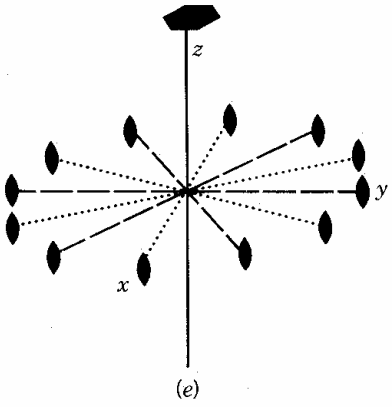




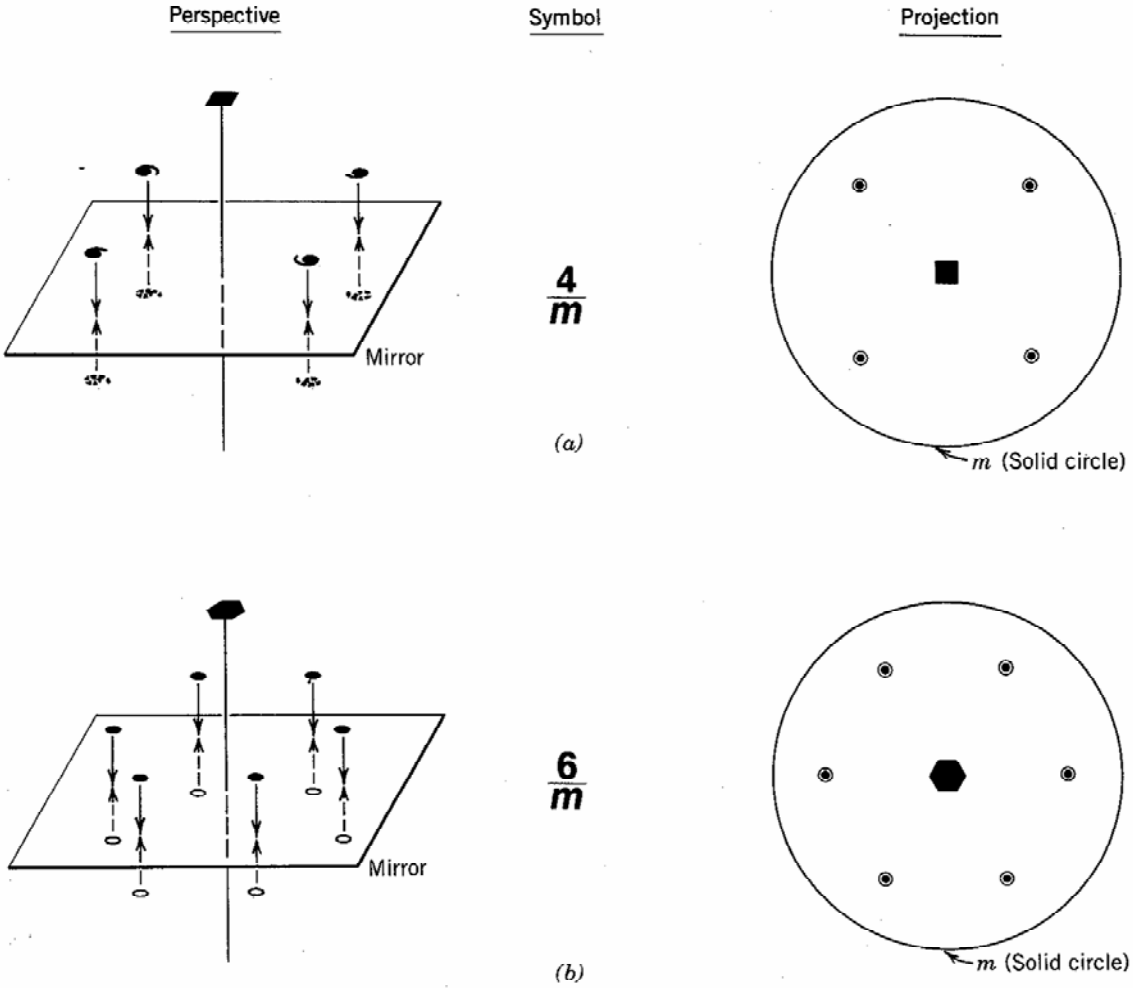


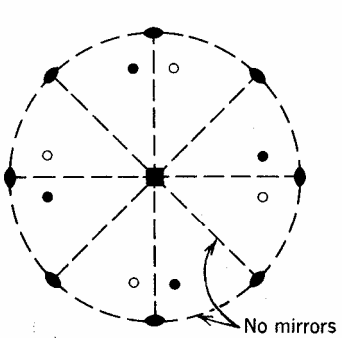






Combinations of rotation axes and mirror planes





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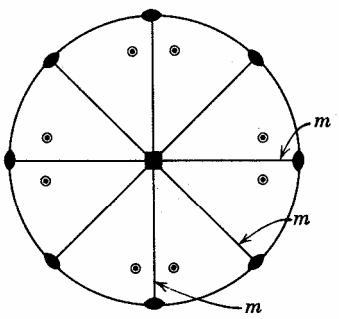
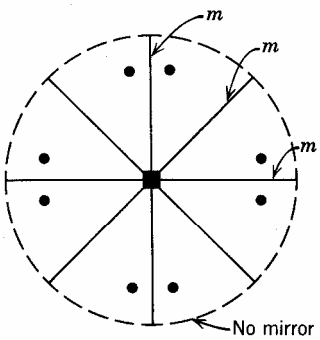
(a)



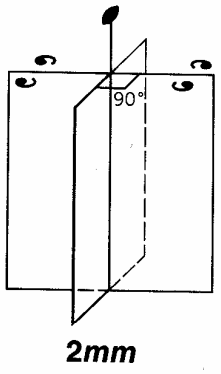
4/m 2/m 2/m

(b)



4mm

(c)



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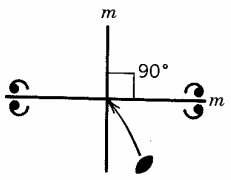

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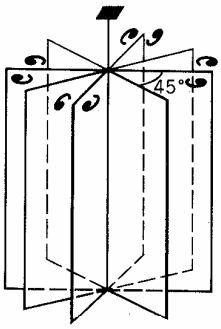

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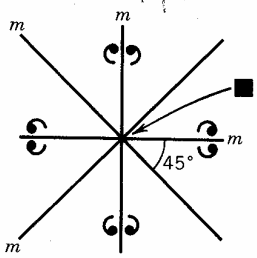

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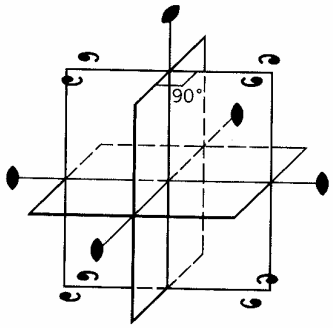
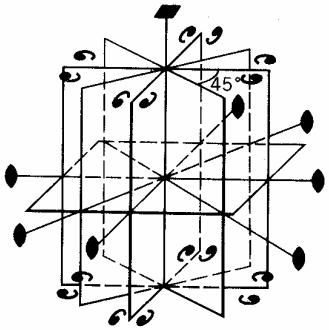


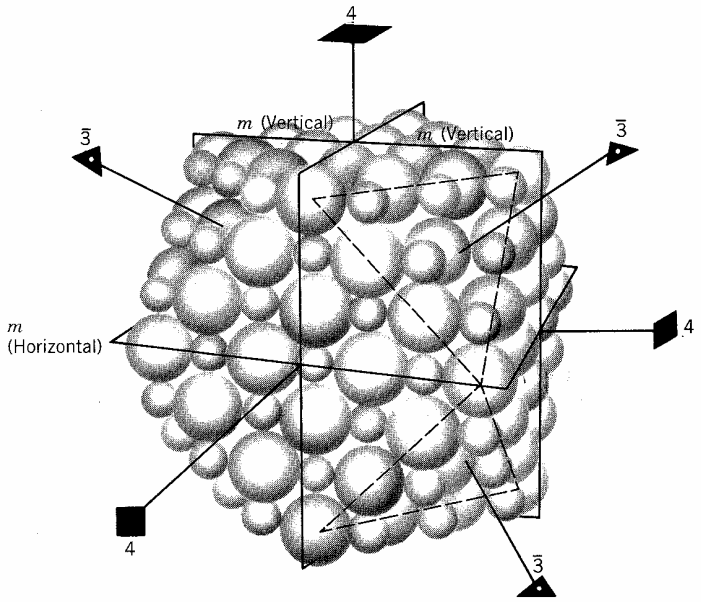
$\frac{2}{m}$ $\frac{2}{m}$ $\frac{2}{m}$

(c)

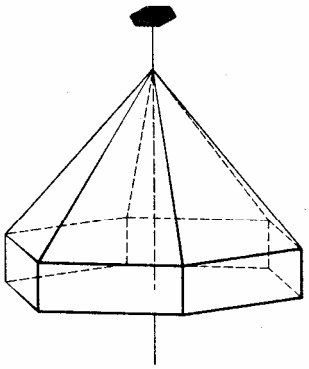


$\frac{4}{m}$ $\frac{2}{m}$ $\frac{2}{m}$

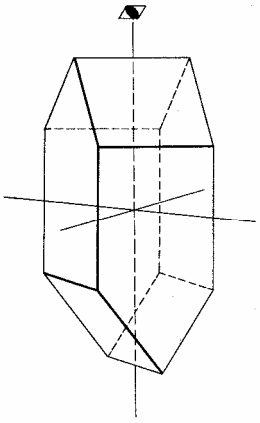
(d)



NaCl structure in cubo-octahedral outline showing square cube faces and triangular octahedral faces



(a)



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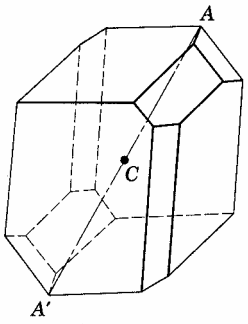

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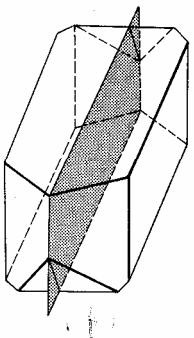

(d)

Point group

Point ➔ symmetry operations leave one particular point, at least, of the pattern unmoved

Group ➔ mathematical theory that allows systematic derivation of all possible and non-identical symmetry combinations.

: 32 possible symmetry combination (without translation)

: 32 crystal classes of which crystal can be assigned on basis of their morphology

: Hermann-Maugin Symbols (notation), International symbols e.g. 2/*m*, 4*mm*, 2/*m*, 4/*m* $\bar{3}$ 2/*m*

Increasing rotational symmetry →					
Rotation axis	1	2	3	4	6
Rotoinversion axis	$\bar{1}$ (= *i*)	$\bar{2}$ (= m)	$\bar{3}$	$\bar{4}$	$\bar{6}$ (= 3/m)
Comb. rotation axes		222	32	422	622
Rotation axis + ⊥ *m*		2/*m*	3/*m* (= $\bar{6}$)	4/*m*	6/*m*
Rotation axis + // *m*		2*mm*	3*m*	4*mm*	6*mm*
Roto + Rotate + *m*			$\bar{3}$2/*m*	$\bar{4}$2/*m*	$\bar{6}$2/*m*
3 Rotation axes + ⊥ *m*		2/*m*2/*m*2/*m*		4/*m*4/*m*4/*m*	6/*m*6/*m*6/*m*
Isometric symmetry		23, 2/m $\bar{3}$		432, $\bar{4}$3*m*	4/*m* $\bar{3}$ 2/*m*

Space groups

: Represent the various ways in which motif can be arranged in space in a homogeneous array.

: Combination of the concepts of 14 Bravais Lattice, 32 Crystal classes, and symmetry operation with translation.

: 230 space groups

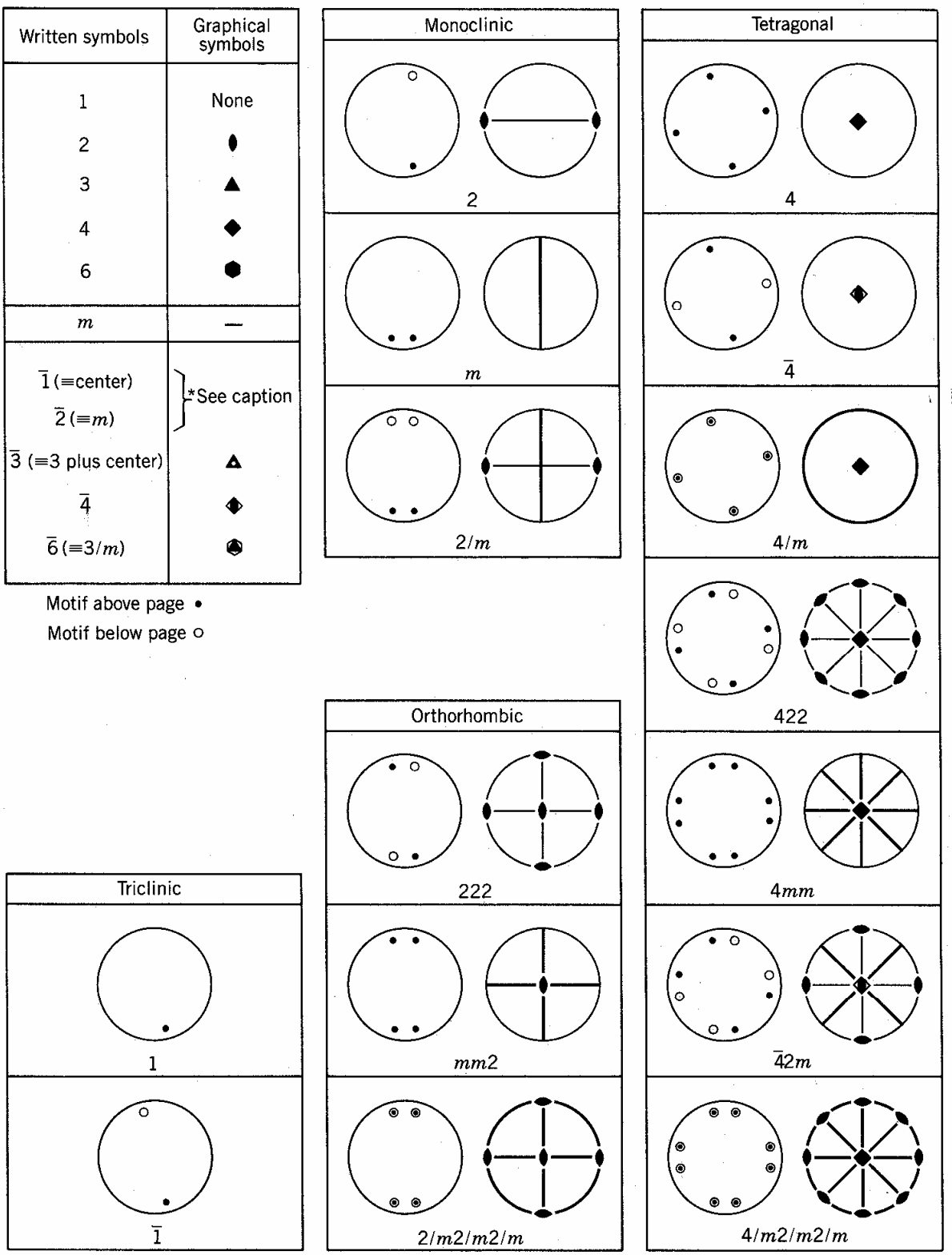

FIG. 2.21. Graphic representation of the distribution of motif units compatible with the symmetry elements of each of the 32 crystal classes (point groups). For all crystal classes, excepting triclinic, there are two circular diagrams, with the left-hand diagram showing the distribution of motif units and the right-hand diagram illustrating the symmetry elements consistent with these motif units. The motif units above the page are equivalent to those below the page, but they are differentiated by dots (above the page) and circles (below the page). The symbols for the symmetry elements are given at the top left corner of the diagram. The presence of a center of symmetry is not shown by any symbol; its presence can be deduced from the arrangement of motif units. Instead of $\bar{2}$ the symbol for a mirror (m) is used. The diagrams for the monoclinic system are shown in what crystallographers refer to as the "second setting," with m vertical (perpendicular to the page) and the 2-fold axis in an east-west orientation. Monoclinic symmetry can also be shown by setting the 2-fold rotation axis perpendicular to the page, and orienting the mirror parallel to the page; this is referred to as the "first setting."

(continued)

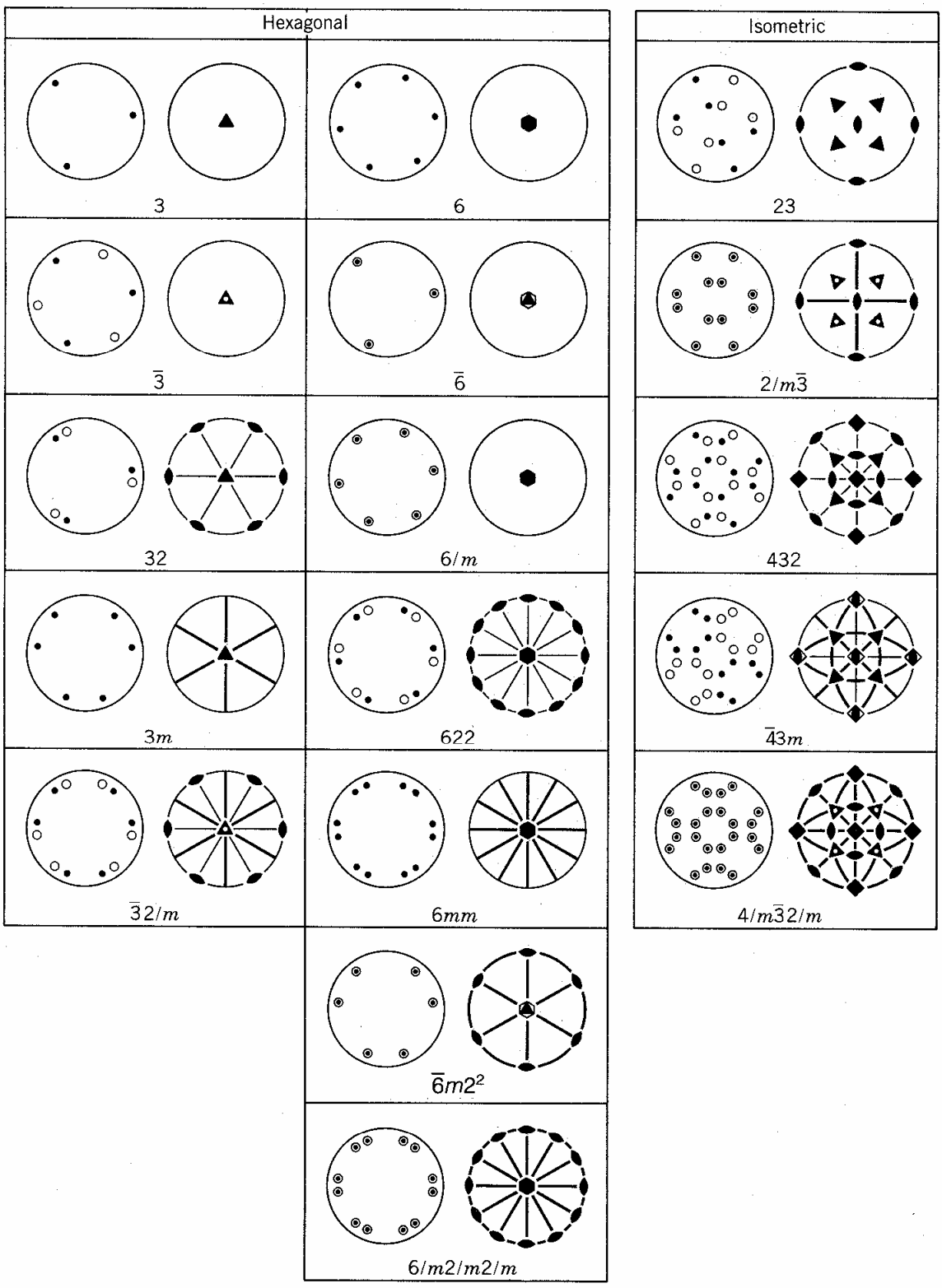

FIG. 2.21. *(continued)*

[2]Because $\bar{6}$ is equivalent to $3/m$, the intersections of the horizontal mirror (perpendicular to the vertical axis) with the vertical mirrors result in 2-fold axes lying in the planes of the vertical mirrors. As such, the traces of the vertical mirrors and the horizontal 2-fold axes are coincident.